Defect-Induced Nucleation in Cubic to Tetragonal Martensites

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Shape memory alloys such as NiTi exhibit interesting mechanical properties due to a diffusionless structural phase transformation from a high temperature (Austenite), in general a cubic, phase to a low temperature (Martensite) tetragonal, orthorhombic or monoclinic phase. This transition is usually first order and is accompanied by a spontaneous strain. The martensitic transition is also responsible for the shape memory effect that refers to the recovery by heating of an apparently permanent deformation undergone below a critical temperature. This property makes shape memory materials suitable for a large number of technological applications. Another important property of shape memory materials is the so-called pseudoelastic behavior that arises due to a reversible stress/strain induced martensitic transformation at a temperature that is higher than the austenite finish temperature of the material. In pseudoelastic deformation, a high temperature cubic austenite phase typically transforms to the martensite under deformation so that there is a plateau in the stress-strain curves. On removing the deformation, the material transforms back to the cubic austenite and the deformation is recovered upon unloading. In fact, some shape memory materials can recover strains of up to 10% under tension, making these materials suitable for actuator applications.

The martensitic transformation results in the formation of a complex microstructure consisting of twin boundaries between the crystallographic variants of the transformation. This microstructure influences the effective mechanical properties of these materials. For example, if a stress is applied to a material in the martensitic phase, there is motion of the twin boundaries as the favored variants grow at the expense of the unfavored variants. Even during pseudoelastic deformation, the strain induced transformation involves nucleation and growth of the martensitic variants. The motion of the domain walls can influence the strain rate dependence of the mechanical response and thus it is important to incorporate this aspect in a theoretical framework. We have theoretically studied the role of microstructural evolution on the mechanical response of shape memory materials, in particular the effects of defect induced heterogeneous nucleation and motion of twin boundaries during cubic to tetragonal deformation of martensite [1].

A number of approaches have been used to model shape memory materials. These include energy minimization techniques that are subject to certain constraints that ensure the integrity of the lattice and micromechanical models that require prior knowledge of the habit planes and their volume fractions. Such techniques have been successful in estimating the recoverable strains for many martensitic transformations. Over the past few years, continuum models based on the Ginzburg-Landau approach have also been used to study the mechanical response of shape memory alloys. The effect of microstructure on the effective stress-strain response has also been simulated using the time-dependent Ginzburg-Landau approach. However, these studies do not consider the strain rate dependence of the stress-strain behavior. We have used a displacement field based dynamical model to study the effect of defects and microstructure on the stress-strain properties of shape memory materials. We have also investigated how microstructural evolution influences the strain rate dependence of the mechanical response [1].

We present 3-D simulations of the microstructure and mechanical response of shape memory alloys undergoing cubic to tetragonal transitions, using FePd as an example. The simulations are based on a nonlinear elastic free-energy in terms of the appropriate strain fields. The dynamics is simulated by force balance equations for the displacement fields with a damping term derived from a dissipation function. Stress-strain properties are investigated using strain loading. Specifically, we have probed the influence of the microstructure on the mechanical response and investigated how the stress-strain behavior changes as a function of strain rate. To illustrate this we obtained through a Ginzburg-Landau simulation the stress-strain curves in the presence of defects. We expected that the defects will nucleate the transformation even before the system is in the unstable region, thereby reducing the stress required to cause the transition. To study defect induced transformation, we simulated the loading process with an initial "quenched" seed of the transformed phase that is embedded in the initial austenite matrix. The total uniaxial strain field in this direction is given by

$$\epsilon_{xx} = \partial u_x / \partial x + \epsilon_{xx}^{applied} + \epsilon_{xx}^{seed}$$

where ϵ_{xx}^{seed} is the strain due to the defect.

This represents an inclusion of a cube of the martensite phase of length L_0 in the austenite matrix. A loading process for this system with strain rate $\gamma = 2.23 \times 10^6/\mathrm{s}$ ($L_0 \sim 24$ nm) is shown in the figure. It shows the stress-strain curve and the spatial distribution of ε_{xx} at points **A, B, C, D**, and **E** on the stress-strain curve. To clearly show the evolution of the microstructure around the defect region, we have displayed two mutually intersecting perpendicular planes that pass through the defect. There is a point on the stress-strain curve where austenite and martensite have the same energy. For strains higher than this critical strain, the nucleation of martensite can take place as martensite has lower energy than the austenite. This nucleation process can be observed by comparing the microstructure at points **B** and **C**. One can see the growth of the martensite domains (regions shaded red) from a seed defect that is embedded in the austenite matrix (regions shaded blue). On further loading, the favored variant grows, as can be observed in the snapshot corresponding to **D**. Eventually, a single variant state of the variant stretched along the x direction is established as can be observed in the snapshot **E**. Notice that the strains in the defect regions are higher (4%) than the bulk value (3%). Even during this loading process, the unfavored variants are also formed. We can also obtain the full microstructures for the three strains ε_{xx}, ε_{yy}, and ε_{zz} corresponding to the point **C**. We found that the magnitude of the distortions along the *y* and *z* directions are smaller than those along the favored *x* direction.

These simulations describe processes at relatively small length (submicron) and time (nanoseconds) scales. Refinement of our scheme to a more coarse grained model in terms of volume fractions of the transformed phase is a possible approach to describing larger length scales.

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[1] R. Ahluwalia, et al., *Acta Mater*. **54** (2006).

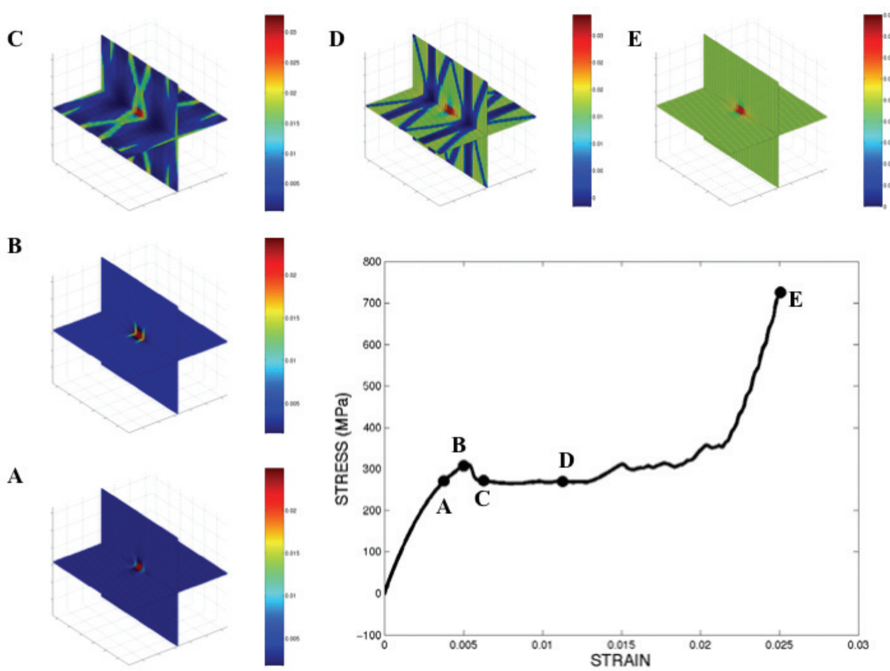

Fig. 1. *The stress-strain curve and the spatial distribution of ε_{xx} at points A, B, C, D, and E on the stress-strain curve.*